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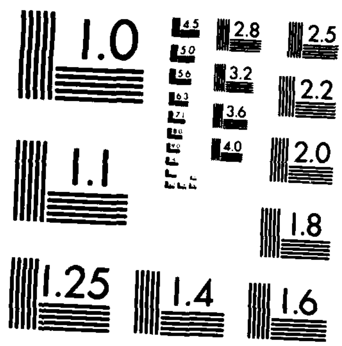

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FINAL REPORT

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"Research on Algorithms for Nonlinear Programming"

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List of Technical Reports & Publications:

SOL 85-1: GILL, Philip E., Walter MURRAY, Michael A. SAUNDERS, G.W. STEWART and Margaret H. WRIGHT. Properties of a Representation of a Basis for the Null Space, February 1985. **Mathematical Programming 33**, 1985, pp. 172-186.

SOL 85-2: GILL, Philip E., Walter MURRAY, Michael A. SAUNDERS, and Margaret H. WRIGHT. Model Building and Practical Aspects of Nonlinear Programming, March 1985. **Computational Mathematical Programming** (K. Schittkowski, ed.) 1985, Springer-Verlag, Berlin, pp. 209-247.

SOL 85-5: LUSTIG, Irvin J. A Practical Approach to Karmarkar's Algorithm, June 1985.

SOL 85-11: GILL, Philip E., Walter MURRAY, Michael A. SAUNDERS, J.A. TOMLIN and Margaret H. WRIGHT. On Projected Newton Barrier Methods for Linear Programming and an Equivalence to Karmarkar's Projective Method, July 1985. **Mathematical Programming 36**, 1986, pp. 183-209.

SOL-86-1: GILL, Philip E., Sven J. HAMMARLING, Walter MURRAY, Michael A. SAUNDERS, G.W. STEWART and Margaret H. WRIGHT. User's Guide for LSSOL (Version 1.0): A Fortran Package for Constrained Linear Least-Squares and Convex Quadratic Programming, January 1986.

SOL-86-2: GILL, Philip E., Walter MURRAY, Michael A. SAUNDERS and Margaret H. WRIGHT. User's Guide for NPSOL (Version 4.0): A Fortran Package for Nonlinear Programming, January 1986.

SOL-86-6: GILL, Philip E., Walter MURRAY, Michael A. SAUNDERS and Margaret H. WRIGHT. Some Theoretical Properties of an Augmented Lagrangian Merit Function, April 1986. Submitted to **SIAM Journal on Numerical Analysis.**

SOL-86-8: GILL, Philip E., Walter MURRAY, Michael A. SAUNDERS and Margaret H. WRIGHT. Maintaining LU Factors of a General Sparse Matrix, May 1986. **Linear Algebra and Its Applications 88/89**, 1987, pp. 239-270.

SOL-86-9: HOYLE, Stephen C. A Single-Phase Method for Quadratic Programming, April 1986.

Scientific Personnel Supported by This Project:

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Degrees Awarded During this Project:

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BRIEF OUTLINE OF RESEARCH FINDINGS

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A considerable effort has been made in this period investigating the "new" algorithm for linear programming of Karmarkar. An extensive theoretical and numerical development of the algorithm has been made. The results of this investigation will be published in the near future. In summary we have shown that Karmarkar's algorithm is a synthesis of a projected Newton method and a log barrier transformation. A separate study of Karmarkar's method by a graduate student has been published [SOL 85-5]. In this report it is shown how certain practical difficulties with Karmarkar's original algorithm can be overcome without any loss of the theoretical properties of the algorithm.

The most efficient algorithms for nonlinear constrained optimization problems use a sequential quadratic programming approach. In certain of these algorithms a projection of the Hessian approximation is recurred. The definition of this projection is via a matrix spanning the null-space of the Jacobian matrix. It is vital for such algorithms that this matrix (whose elements are functions) have certain continuity properties. In report SOL 85-1 we show how matrices spanning the null-space may be generated efficiently.

Optimization almost always involves an interactive process between defining the problem (model) and its solution. In report SOL 85-2 this symbiotic relationship is discussed.

BRIEF OUTLINE OF RESEARCH FINDINGS

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July 1, 1985 - December 31, 1985

In the thesis work of Stephen Hoyle a single phase active set method has been developed. It differs from other active-set methods in that the current iterate may violate constraints in the working set. One consequence of allowing violations is that the Kuhn-Tucker equations may become linearly dependent. A key finding of the research was how to circumvent such singularities. It is of particular importance that the techniques developed are applicable to large-scale problems.

Our work on interior point methods for linear programming has continued. The report on this work, SOL 85-11, has been in great demand. A prototype algorithm has been developed and tested on a selection of medium to large-scale problems. The initial results are extremely encouraging. Current research efforts are being directed at improving the efficiency of solving the linear least squares problem that occurs at each iteration of the method.

Among the topics discussed in the paper "Model Building and Practical Aspects of Nonlinear Programming", is how the QP subproblems posed at each iteration of an SQP method can be solved with high efficiency by utilizing information available from the previous iteration.

BRIEF OUTLINE OF RESEARCH FINDINGS

ARO Contract: DAAG29-84-K-0156

1 January 1986 - 30 June 1986

During the current period a larger number of reports were published than usual. Much of the work contained in the reports had been in progress over several years. For example, the report SOL 86-9 is the Ph.D. thesis of Stephen Hoyle. This report may be viewed as a first step in developing a general purpose QP algorithm for large-scale problems.

The report 86-8 describes a set of algorithms for computing and modifying the LU factors of a sparse rectangular matrix. Such algorithms form the basic building blocks, not only of algorithms for large-scale optimization, but also for many other areas of scientific computing.

The reports 86-1 and 86-2 are users guides for the fortran packages LSSOL and NPSOL respectively. Unlike the package QPSOL (SOL 84-6), the routine LSSOL takes specific advantage of the problem being convex. Moreover, the problem may be stated in the form of a least squares. Consequently, LSSOL is able to solve considerably worst conditioned problems than QPSOL. Ill conditioning is a common feature of least square problems. The new version of NPSOL incorporates LSSOL in addition to a number of other important changes. Perhaps the most significant change is that gradients are no longer an essential requirement. Work is continuing on NPSOL. Currently alternative quasi-Newton updates are being investigated.

In report 86-6 the theoretical foundation of the merit function used in NPSOL is given.

BRIEF OUTLINE OF RESEARCH FINDINGS

ARO Contract: DAAG29-84-K-0156
1 July 1986 - 31 December 1986

The research on numerical optimization has been in two principal areas. First, work has continued on the development and implementation of reliable algorithms for the solution of constrained least-squares and quadratic programming problems.

One of the most serious questions in the construction of methods for constrained least-squares estimation is the treatment of singularity in the data matrix. Practical problems arising in statistical estimation, robotics and control invariably have singular or ill-conditioned data matrices. These matrices may cause serious problems for numerical algorithms. Algorithms must be able to solve singular problems reliably and efficiently.

One of the most widely-used methods for singular least-squares problems is due to Stoer (On the numerical solution of constrained least-squares problems", SIAM J. on Numerical Analysis 8, 382-411, 1971). In Stoer's method, the original data matrix is overwritten by the so-called <u>complete orthogonal factorization</u> of a reduced matrix related to the projected Hessian. The orthogonal factorization is then updated as constraints enter or leave the working set. At each iteration, the updating procedure requires some procedure for estimating the rank of the reduced matrix. This decision implicitly defines some part of the factorization as being "negligible" and small elements are discarded. Unfortunately, a guaranteed strategy for determining the numerical "rank" of a matrix is not possible, since the crucial decision about when a quantity is"negligible" depends on the problem. If a wrong decision is made about the rank and information is erroneously discarded, the computed solution may be that of a problem that differs considerably from the original.

A new method for constrained least-squares and positive semi-definite quadratic programming has been developed that is less susceptible to the problems of rank determination. In the new method, a decision about rank does not imply that small elements in a reduced matrix are assumed to be zero. As a consequence, the problem does not implicitly change as the iterations proceed. Work is in progress on an SOL report describing the theoretical details of the algorithm. The new method has been implemented in an updated version of the SOL Fortran package for constrained least-squares and quadratic programming.

The second area of active research concerns the development of techniques for generating test problems for linear programming, quadratic programming and constrained least-squares.

A key tool in the development of algorithms is the availability of a pool of realistic non-trivial test problems. The theoretical analysis of algorithms yields much information concerning efficiency and numerical stability. However, the ultimate test is how the algorithm performs in practical situations. An algorithm should be tested not only in its final form, but also throughout its development stages. In many cases, the only way to choose between seemingly equivalent strategies is to select that which is the most effective.

During the last contract period, a problem generator has been developed for positive-definite and indefinite quadratic programming.

The generator has a number of unique features. First, it requires only minimal input data, the dimension of the problem, the number of constraints active at the solution, and the spread of singular values of the constraints and the Hessian matrix of second derivatives. Second, it is possible to specify the range of singular values of certain key matric projections that occur in the bounds on the absolute perturbation of the solution and multipliers induced by perturbations in the data.

We anticipate that the availability of the problem generator will have a major impact on research in constrained least-squares and quadratic programming st SOL and other centers of research.

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The following reports ~~contain~~ containing the research results:
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